=> fil reg FILE 'REGISTRY' ENTERED AT 14:12:34 ON 11 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9 DICTIONARY FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

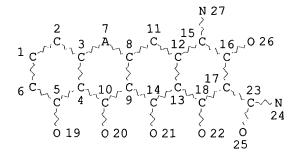
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> d sta que 148 L1 STF



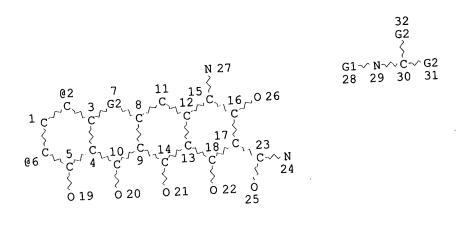
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GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L3 5035 SEA FILE=REGISTRY SSS FUL L1

L4 ST



VAR G1=2/6 VAR G2=O/S/N/C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE
L6 696 SEA FILE=REGISTRY SUB=L3 SSS FUL L4
L7 STR 32

VAR G1=2/6
VAR G2=O/S/N/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC 1 NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE L8 630 SEA FILE=REGISTRY SUB=L6 SSS FUL L7 L10 STR (1) subset

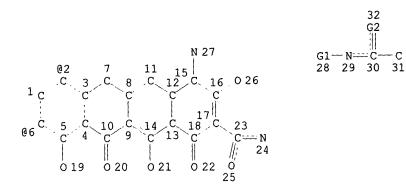
28 29 30 31

G2

G2 5

G1-N-C

New search Unsut



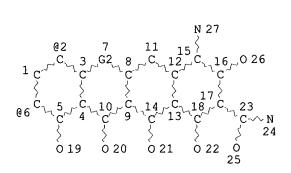
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GRAPH ATTRIBUTES:

RSPEC 1 NUMBER OF NODES IS 32

STEREO L11 L12 L15 L16	115 9	SEA FILE=REGISTRY SUB=L8 SSS FUL L10 SEA FILE=REGISTRY ABB=ON PLU=ON L8 NOT L11 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 SEA FILE=HCAPLUS ABB=ON PLU=ON (PARATEK/PA OR PARATEK/CS OR
		"PARATEK INC ABERDEEN MD 21001 USA"/CS OR "PARATEK MICROWAVE INC USA"/PA OR "PARATEK MICROWAVE INC USA"/CS OR "PARATEK PHARACEUTICALS INC"/PA OR "PARATEK PHARACEUTICALS INC"/CS OR "PARATEK PHARMACEUTICALS BOSTON MA 02111 USA"/CS OR "PARATEK PHARMACEUTICALS INC"/PA OR "PARATEK PHARMACEUTICALS INC"/CS OR "PARATEK PHARMACEUTICALS INC BOSTON MA 02111 USA"/CS OR "PARATEK PHARMACEUTICATS INC BOSTON MA 02111 USA"/CS)
L17	78	SEA FILE=HCAPLUS ABB=ON PLU=ON ("NELSON M"/AU OR "NELSON M L"/AU)
L18	35	SEA FILE=HCAPLUS ABB=ON PLU=ON ("NELSON MARK"/AU OR "NELSON MARK LESLIE"/AU OR "NELSON MARK LOGE"/AU OR "NELSON MARK LOUIS"/AU)
L19	125	SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEVY S"/AU OR "LEVY SB"/AU)
L20	221	SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEVY STUARD B"/AU OR "LEVY STUART"/AU OR "LEVY STUART B"/AU)
L21	24	SEA FILE=HCAPLUS ABB=ON PLU=ON ("FRECHETTE R"/AU OR "FRECHETTE R F"/AU OR "FRECHETTE ROGER F"/AU)
L22	6	SEA FILE=HCAPLUS ABB=ON PLU=ON ("BOWSER T"/AU OR "BOWSER TODD"/AU OR "BOWSER TODD E"/AU OR "BOWSER TODD EVERETT"/AU)
L23	162	SEA FILE=HCAPLUS ABB=ON PLU=ON ("ISMAIL M"/AU OR "ISMAIL M Y"/AU OR "ISMAIL M YEHIA"/AU OR "ISMAIL M YEHIO"/AU)
L24	13	SEA FILE=HCAPLUS ABB=ON PLU=ON "ISMAIL MOHAMED"/AU
L25	2	SEA FILE=HCAPLUS ABB=ON PLU=ON "ISMAIL MOHAMED Y"/AU
L26	6	SEA FILE=HCAPLUS ABB=ON PLU=ON "ISMAIL MOHAMMAD"/AU
L27	4	SEA FILE=HCAPLUS ABB=ON PLU=ON "ISMAIL MUHAMMAD"/AU
L28	10677	SEA FILE=HCAPLUS ABB=ON PLU=ON (TUFT/PA OR TUFT/CS OR "TUFT
		S COLL MA"/CS OR "TUFT S UNIV MED SCHOOL BOSTON MA"/CS OR "TUFT UNIV MEDFORD MA"/CS OR TUFTS/PA OR TUFTS/CS)
L29	3	SEA FILE=HCAPLUS ABB=ON PLU=ON L15 AND (L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR L28)
L30	24	SEA FILE=HCAPLUS ABB=ON PLU=ON "NELSON MARK L"/AU
L31	1	SEA FILE=HCAPLUS ABB=ON PLU=ON "PRECHETTE ROGER"/AU

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L32
             3 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 AND (L30 OR L31)
             3 SEA FILE=HCAPLUS ABB=ON PLU=ON (L29 OR L32)
L33
L34
             3 SEA FILE=HCAPLUS ABB=ON PLU=ON
                                                L3 AND L33
L35
                SEL PLU=ON L34 1- RN:
                                            394 TERMS
            394 SEA FILE=REGISTRY ABB=ON
L36
                                         PLU=ON L35
                                         PLU=ON L3 AND L36
            367 SEA FILE=REGISTRY ABB=ON
L37
L38
            92 SEA FILE=REGISTRY ABB=ON
                                         PLU=ON L37 AND L6
L39
            275 SEA FILE=REGISTRY ABB=ON
                                        PLU=ON L37 NOT L38
L40
            19 SEA FILE=REGISTRY ABB=ON PLU=ON L39 AND (C31H33BRN4O9 OR
               C32H36N4O9 OR C31H42N4O9 OR C28H36N4O10 OR C28H35N3O9 OR
               C31H34N4O9 OR C30H4ON4O9 OR C29H36N4O9 OR C32H34F3N5O9 OR
               C33H40N608 OR C33H37N509 OR C26H31N309 OR C32H35N5010 OR
               C31H33FN409 OR C33H37N309 OR C27H31CL3N409 OR C31H33CLN409)
L41
             1 SEA FILE=REGISTRY ABB=ON PLU=ON L40 AND C32H36N4O9 AND 6/NR
                                        PLU=ON L40 NOT L41
L42
             18 SEA FILE=REGISTRY ABB=ON
L43
             88 SEA FILE=REGISTRY ABB=ON PLU=ON L38 NOT (389625-00-7 OR
                389139-15-5 OR 365277-33-4 OR 161320-33-8)
L44
            106 SEA FILE=REGISTRY ABB=ON PLU=ON (L42 OR L43)
L45
               STR
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32 Q \$ G1~N~C~Q 28 29 30 31

VAR G1=2/6
VAR G2=O/S/N/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE

L46 120 SEA FILE=REGISTRY SUB=L6 SSS FUL L45

L48 139 SEA FILE=REGISTRY ABB=ON PLU=ON (L44 OR L46)

=> d his

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L1
                 STR
             50 S L1
L2
L3
           5035 S L1 FUL
                 SAV L3 GERSTL823/A
L.4
                 STR L1
L5
             29 S L4 SAM SUB=L3
            696 S L4 FUL SUB≈L3
L6
                 SAV L6 GERSTL823A/A
1.7
                 STR L4
^{18}
            630 S L7 FUL SUB=L6
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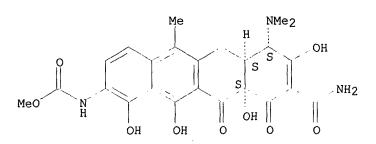
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SAV L8 GERSTL832B/A
L9
             66 S L6 NOT L8
L10
                STR L7
            515 S L10 FUL SUB=L8
L11
                SAV L11 GERSTL823C/A
L12
            115 S L8 NOT L11
L13
                STR L10
              0 S L13 FUL SUB=L6
L14
                SAV L14 GERSTL832D/A
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L15
              9 S L12
                E PARATEK/PA, CS
             12 S E3-E14
L16
                E NELSON M/AU
             78 S E3, E20
L17
                E NELSON MARK/AU
L18
             35 S E3, E16-E18
                E LEVY S/AU
            125 S E3,E5
L19
                E LEVY STU/AU
            221 S E4-E6
L20
                E FRECHETTE R/AU
             24 S E3, E4, E8, E9
L21
                E BOWSER T/AU
L22
              6 S E3, E9-E11
                E ISMAIL M/AU
            162 S E3, E30-E32
L23
                E ISMAIL MOH/AU
             13 S E7
L24
L25
              2 S E27
L26
              6 S E28
L27
              4 S E52
                E TUFT/PA, CS
L28
          10677 S E3-E7, E12, E13
L29
              3 S L15 AND L16-L28
                E NELSON MARK L/AU
             24 S E3
L30
                E PRECHETTE R/AU
              1 S E4
T.31
L32
              3 S L15 AND L30, L31
L33
              3 S L29, L32
L34
              3 S L3 AND L33
     FILE 'REGISTRY' ENTERED AT 13:41:48 ON 11 FEB 2002
     FILE 'HCAPLUS' ENTERED AT 13:41:48 ON 11 FEB 2002
                 SET SMARTSELECT ON
L35
            SEL L34 1- RN:
                                  394 TERMS
                 SET SMARTSELECT OFF
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L36
            394 S L35
L37
            367 S L3 AND L36
L38
             92 S L37 AND L6
            275 S L37 NOT L38
L39
             19 S L39 AND (C31H33BRN4O9 OR C32H36N4O9 OR C31H42N4O9 OR C28H36N4
L40
              1 S L40 AND C32H36N4O9 AND 6/NR
L41
L42
             18 S L40 NOT L41
             88 S L38 NOT (389625-00-7 OR 389139-15-5 OR 365277-33-4 OR 161320-
L43
            106 S L42, L43
L44
                 STR L4
L45
            120 S L45 FUL SUB=L6
L46
                 SAV L46 GERSTL832E/A
                 DEL GERSTL832E/A
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SAV L46 GERSTL823E/A

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33 S L46 NOT L44
L47
            139 S L44, L46
L48
                SAV L48 GERSTL823F/A
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              0 S L48
L49
     FILE 'HCAPLUS' ENTERED AT 14:10:28 ON 11 FEB 2002
L50
              9 S L48
              3 S L50 AND (TUFT? OR PARAT?)/PA,CS
L51
              3 S L50 AND (NELSON M? OR LEVY S? OR FRECHETTE R? OR BOWSER T? OR
L52
              3 S L51, L52
L53
              6 S L50 NOT L53
L54
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              8 S L48
L55
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CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
FILE 'USPAT2' ENTERED AT 14:12:45 ON 11 FEB 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)
=> d 155 bib abs hitrn fhitstr tot
     ANSWER 1 OF 8 USPATFULL
T.55
AN
       2000:174627 USPATFULL
       Tetracycline derivatives
TΙ
       Vu, Chi Bao, Chestnut Hill, MA, United States
IN
       Pfizer Inc, New York, NY, United States (U.S. corporation)
PA
                                20001226
       US 6165999
PΙ
       WO 9634852 19961107
                                19980223 (8)
       US 1998-945775
ΑI
                                19960417
       WO 1996-IB335
                                19980223
                                          PCT 371 date
                                19980223 PCT 102(e) date
DT
       Utility
       Granted
FS
       Primary Examiner: Barts, Samuel
EXNAM
       Richardson, Peter C., Ginsburg, Paul H., Levine, Jacob M.
LREP
       Number of Claims: 19
CLMN
       Exemplary Claim: 1
ECL
       No Drawings
DRWN
LN.CNT 2428
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The present invention relates to novel tetracycline derivatives, to
AΒ
        intermediates used in their preparation, to pharmaceutical compositions
       containing them and to their medicinal use.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 TT
     184593-35-9P
         (prepn. of antibacterial tetracycline derivs.)
      184593-34-8P 184593-37-1P 184593-41-7P
 IT
       184593-66-6P 184593-69-9P
         (prepn. of antibacterial tetracycline derivs.)
     184593-35-9P
 ΙT
         (prepn. of antibacterial tetracycline derivs.)
      184593-35-9 USPATFULL
 RN
      Carbamic acid, [9-(aminocarbonyl)-7-(dimethylamino)-6,6a,7,10,10a,11-
 CN
        hexahydro-1,8,10a,12-tetrahydroxy-5-methyl-10,11-dioxo-2-naphthacenyl]-,
        methyl ester, [6aS-(6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX
```

NAME)

Absolute stereochemistry.





```
L55 ANSWER 2 OF 8 USPATFULL
       1999:37286 USPATFULL
AN
ΤI
       7-(substituted)-8-(substituted)-9-(substitued amino)-6-demethyl-6-
       deoxytetracyclines
       Sum, Phaik-Eng, Pomona, NY, United States
IN
       Lee, Ving J., Monsey, NY, United States
       Hlavka, Joseph J., Tuxedo Park, NY, United States Testa, Raymond T., Cedar Grove, NJ, United States
       American Cyanamid Company, Wayne, NJ, United States (U.S. corporation)
PA
                                19990323
PI
       US 5886175
       US 1994-352310
ΑI
                                19941208 (8)
       Division of Ser. No. US 1994-214992, filed on 21 Mar 1994, now abandoned
RLI
       which is a continuation of Ser. No. US 1992-928598, filed on 13 Aug
       1992, now abandoned
DT
       Utility
       Granted
FS
       Primary Examiner: Kestler, Kimberly J.
EXNAM
LREP
       Szatkowski, T. S.
CLMN
       Number of Claims: 8
       Exemplary Claim: 1
ECL
DRWN
       No Drawings
LN.CNT 8288
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The invention provides compounds of the formulas ##STR1## which are
AB
       useful as intermediates for the preparation of 6-demethyl-6-
       deotetracycline antibiotic agents.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
ΙT
     157579-07-2P 157579-18-5P 157579-22-1P
      157579-23-2P 157579-26-5P 157579-28-7P
      157579-29-8P 157579-30-1P 157579-31-2P
      157579-36-7P 157579-37-8P
        (prepn. of, as antibiotic)
IT
    157579-07-2P
        (prepn. of, as antibiotic)
     157579-07-2 USPATFULL
     Carbamic acid, [9-(aminocarbonyl)-3-chloro-7-(dimethylamino)-
CN
       5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-
       naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alp
       ha.)]- (9CI) (CA INDEX NAME)
```

```
L55
    ANSWER 3 OF 8 USPATFULL
       96:55871 USPATFULL
AN
       7-substituted-9-substituted amino-6-demethyl-6-deoxytetracyclines
TТ
IN
       Hlavka, Joseph J., Tuxedo Park, NY, United States
       Sum, Phaik-Eng, Pomona, NY, United States
       Gluzman, Yakov, Upper Saddle River, NJ, United States
       Lee, Ving J., Monsey, NY, United States
       Ross, Adma A., Airmont, NY, United States
       American Cyanamid Company, Wayne, NJ, United States (U.S. corporation)
PA
                               19960625
PΙ
       US 5530117
                               19950531 (8)
       US 1995-455923
AΤ
       Division of Ser. No. US 1994-286096, filed on 4 Aug 1994 which is a
RLI
       continuation of Ser. No. US 1992-926091, filed on 13 Aug 1992, now
       abandoned which is a continuation-in-part of Ser. No. US 1991-771576,
       filed on 4 Oct 1991, now abandoned
DT
       Utility
FS
       Granted
       Primary Examiner: Prior, Kimberly J.
EXNAM
       Szatkowski, T. S.
LREP
       Number of Claims: 8
CLMN
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 7954
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The disclosure is drawn to novel 7-substituted-9-(substituted
AΒ
       amino)-6-demethyl-6-deoxytetracycline compounds. These compounds are
       useful to treat infections caused by a wide spectrum of bacterial
       organisms, including those which are resistant to tetracycline.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     150231-22-4P 150231-23-5P 150251-75-5P
      150251-76-6P 150251-77-7P 150251-78-8P
      150521-69-0P 150521-70-3P
        (prepn. of, as antibacterial)
TT
    150231-22-4P
        (prepn. of, as antibacterial)
     150231-22-4 USPATFULL
RN
     Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-
CN
       5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-
       dioxo-2-naphthacenyl]-, 2-(diethylamino)ethyl ester, monohydrochloride,
       [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA
       INDEX NAME)
```

● HCl

```
ANSWER 4 OF 8 USPATFULL
L55
ΑN
       96:55747 USPATFULL
TΙ
       Method for treating bacterial infection with novel 7-substituted-9-
       substituted amino 6-demethyl-6-deoxytetracyclines
IN
       Hlavka, Joseph J., Tuxedo Park, NY, United States
       Sum, Phaik-Eng, Pomona, NY, United States
       Gluzman, Yakov, Upper Saddle River, NJ, United States
       Lee, Ving J., Monsey, NY, United States
       Ross, Adma A., Airmont, NY, United States
       American Cyanamid Company, Wayne, NJ, United States (U.S. corporation)
PΑ
PT
       US 5529990
                               19960625
                               19950531 (8)
       US 1995-455446
ΑI
       Division of Ser. No. US 1994-286096, filed on 4 Aug 1994 which is a
RLI
       continuation of Ser. No. US 1992-926091, filed on 13 Aug 1992, now
       abandoned which is a continuation-in-part of Ser. No. US 1991-771576,
       filed on 4 Oct 1991, now abandoned
DT
       Utility
FS
       Granted
EXNAM
       Primary Examiner: Prior, Kimberly J.
       Szatkowski, T. S.
LREP
CLMN
       Number of Claims: 2
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 7061
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The disclosure is drawn to a method of using novel 7-substituted-9-
AB
       (substituted amino)-6-demethyl-6-deoxytetracycline compounds to treat
       infections caused by a wide spectrum of bacterial organisms, including
       those which are resistant to tetracycline.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT
     150231-22-4P 150231-23-5P 150251-75-5P
      150251-76-6P 150251-77-7P 150251-78-8P
      150521-69-0P 150521-70-3P
        (prepn. of, as antibacterial)
IT
    150231-22-4P
        (prepn. of, as antibacterial)
     150231-22-4 USPATFULL
RN
     Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-
CN
       5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-
       dioxo-2-naphthacenyl]-, 2-(diethylamino)ethyl ester, monohydrochloride,
       [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA
       INDEX NAME)
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HC1

```
ANSWER 5 OF 8 USPATFULL
L55
AN
       96:36549 USPATFULL
       7-(substituted)-8-(substituted)-9-(substituted amino)-6-demethyl-6-
TI
       deoxytetracyclines
       Sum, Phaik-Eng, Pomona, NY, United States
IN
       Lee, Ving J., Monsey, NY, United States
       Hlavka, Joseph J., Tuxedo Park, NY, United States
       Testa, Raymond T., Cedar Grove, NJ, United States
       American Cyanamid Company, Wayne, NJ, United States (U.S. corporation)
PA
PΙ
       US 5512553
                               19960430
ΑI
       US 1995-454966
                               19950531 (8)
       Division of Ser. No. US 1994-214992, filed on 21 Mar 1994, now patented,
RLI
       Pat. No. US 5430162 which is a continuation of Ser. No. US 1992-928598,
       filed on 13 Aug 1992
DT
       Utility
       Granted
FS
       Primary Examiner: Goldberg, Jerome D.
EXNAM
LREP
       Szatkowski, T. S.
       Number of Claims: 1
CLMN
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 6597
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The invention provides compounds of formula ##STR1## wherein X, R and
AB
       R.sup.1 are defined in the specification. These compounds are useful as
       antibiotic agents.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     157579-07-2P 157579-18-5P 157579-22-1P
      157579-23-2P 157579-26-5P 157579-28-7P
      157579-29-8P 157579-30-1P 157579-31-2P
      157579-36-7P 157579-37-8P
        (prepn. of, as antibiotic)
   157579-07-2P
IT
        (prepn. of, as antibiotic)
     157579-07-2 USPATFULL
RN
     Carbamic acid, [9-(aminocarbonyl)-3-chloro-7-(dimethylamino)-
CN
       5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-
       naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alp
       ha.) - (9CI)
                    (CA INDEX NAME)
```

```
L55
     ANSWER 6 OF 8 USPATFULL
       96:17091 USPATFULL
ΑN
TI
       7-(substituted-9-(substituted amino)-6-demethyl-6-deoxytetracyclines
IN
       Sum, Phaik-Eng, Pomona, NY, United States
       Lee, Ving J., Monsey, NY, United States
       Hlavka, Joseph J., Tuxedo Park, NY, United States
       Testa, Raymond T., Cedar Grove, NJ, United States
       American Cyanamid Company, Wayne, NJ, United States (U.S. corporation)
PA
                                19960227
PΙ
       US 5495018
ΑI
       US 1994-352407
                                19941208 (8)
       Division of Ser. No. US 1994-214992, filed on 21 Mar 1994, now abandoned
RLI
       which is a continuation of Ser. No. US 1992-928598, filed on 13 Aug
       1992, now abandoned
DT
       Utility
FS
       Granted
EXNAM
       Primary Examiner: Kestler, Kimberly J.
LREP
       Szatkowski, T. S.
CLMN
       Number of Claims: 12
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 7937
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB
       The invention provides compounds of the formulas ##STR1## which are
       useful as intermediates for the preparation of 6-demethyl-6-
       deotetracycline antibiotic agents.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
ΙT
     157579-07-2P 157579-18-5P 157579-22-1P
      157579-23-2P 157579-26-5P 157579-28-7P
      157579-29-8P 157579-30-1P 157579-31-2P
      157579-36-7P 157579-37-8P
        (prepn. of, as antibiotic)
    157579-07-2P
IT
        (prepn. of, as antibiotic)
RN
     157579-07-2 USPATFULL
CN
     Carbamic acid, [9-(aminocarbonyl)-3-chloro-7-(dimethylamino)-
       5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-
       naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alp
       ha.)]- (9CI) (CA INDEX NAME)
```

L55 ANSWER 7 OF 8 USPATFULL 96:16980 USPATFULL ΑN TΤ 7-substituted-9-substituted amino-6-demethyl-6-deoxytetracyclines IN Hlavka, Joseph J., Tuxedo Park, NY, United States Sum, Phaik-Eng, Pomona, NY, United States Gluzman, Yakov, Upper Saddle River, NJ, United States Lee, Ving J., Monsey, NY, United States Ross, Adma A., Airmont, NY, United States PA American Cyanamid Company, Wayne, NJ, United States (U.S. corporation) ΡI US 5494903 19960227 US 1994-286096 19940804 (8) AΙ Continuation of Ser. No. US 1992-926091, filed on 13 Aug 1992, now RLI abandoned which is a continuation-in-part of Ser. No. US 1991-771576, filed on 4 Oct 1991, now abandoned DT Utility FS Granted Primary Examiner: Kestler, Kimberly J. EXNAM LREP Szatkowski, T. S. Number of Claims: 98 CLMN ECL Exemplary Claim: 1 DRWN No Drawings LN.CNT 7074 CAS INDEXING IS AVAILABLE FOR THIS PATENT. The invention is drawn to 7-substituted-9-(substituted amino)-6-demethyl-6-deoxytetracycline compounds of the formula ##STR1## wherein R, X, R.sup.5 and R.sup.6 are defined in the specification. The compounds of the invention are useful as broad spectrum antibiotics. CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 150231-22-4P 150231-23-5P 150251-75-5P 150251-76-6P 150251-77-7P 150251-78-8P 150521-69-0P 150521-70-3P (prepn. of, as antibacterial)

T 150231-22-4P

(prepn. of, as antibacterial)

RN 150231-22-4 USPATFULL

CN Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, 2-(diethylamino)ethyl ester, monohydrochloride, [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

L55 ANSWER 8 OF 8 USPATFULL AN 95:60497 USPATFULL

TI 7-(substituted)-8-(substituted)-9-substituted amino)-6-demethyl-6-deoxytetracyclines

IN Sum, Phaik-Eng, Pomona, NY, United States

Lee, Ving J., Monsey, NY, United States Hlavka, Joseph J., Tuxedo Park, NY, United States Testa, Raymond T., Cedar Grove, NJ, United States American Cyanamid Company, Wayne, NJ, United States (U.S. corporation) PΑ PΙ US 5430162 19950704 US 1994-214992 19940321 (8) ΑI DCD 20120530 Continuation of Ser. No. US 1992-928598, filed on 13 Aug 1992, now RLI abandoned DT Utility Granted FS Primary Examiner: Richter, Johann; Assistant Examiner: Kestler, Kimberly EXNAM Szatkowski, T. S. LREP Number of Claims: 4 CLMN Exemplary Claim: 1 ECL DRWN No Drawings LN.CNT 6553 CAS INDEXING IS AVAILABLE FOR THIS PATENT. The invention provides compounds of formula ##STR1## wherein X, R and AB R.sup.1 are defined in the specification. These compounds are useful as antibiotic agents. CAS INDEXING IS AVAILABLE FOR THIS PATENT. 157579-07-2P 157579-18-5P 157579-22-1P IΤ 157579-23-2P 157579-26-5P 157579-28-7P 157579-29-8P 157579-30-1P 157579-31-2P 157579-36-7P 157579-37-8P (prepn. of, as antibiotic) 157579-07-2P IT (prepn. of, as antibiotic) RN 157579-07-2 USPATFULL Carbamic acid, [9-(aminocarbonyl)-3-chloro-7-(dimethylamino)-CN 5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alp ha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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FILE COVERS 1907 - 8 Feb 2002 VOL 136 ISS 7 FILE LAST UPDATED: 30 Jan 2002 (20020130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

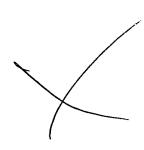
CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> d 154 bib abs hitrn fhitstr tot

GΙ

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ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2002 ACS
    1997:327 HCAPLUS
DN
    126:31223
    Preparation of novel tetracycline derivatives
TΤ
IN
    Vu, Chi Bao
PA
    Pfizer, Inc., USA; Vu, Chi Bao
    PCT Int. Appl., 96 pp.
SO
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
                      ____
                            _____
ΡI
    WO 9634852
                      A1
                            19961107
                                           WO 1996-IB335
                                                             19960417
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        RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
    CA 2219277
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                            19961121
                                                             19960417
    AU 693013
                       B2
                            19980618
    EP 823893
                       A1
                            19980218
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                                                             19960417
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    JP 11504916
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                                                             19960417
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                            20001226
                                           US 1998-945775
                                                             19980223
                       Α
PRAI US 1995-433102
                       Α
                            19950503
    WO 1996-IB335
                            19960417
OS
    MARPAT 126:31223
```



AB Novel tetracycline derivs. I and II (R3 = MeS, alkoxy, amino, substd. to form guanidino, amido, carboxamido; R8 = carboxamido) were prepd. as antibiotics for tetracycline resistant bacteria. Thus, 9-aminoanhydrotetracycline was acetylated with BrCH2COBr to form II (R3 = BrCH2CO, R8 = CONH2).

II

Ι

- IT 184593-35-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
- (prepn. of antibacterial tetracycline derivs.)

 IT 184593-34-8P 184593-37-1P 184593-41-7P

 184593-66-6P 184593-69-9P

 REPROSE (Properties of the properties of the properties

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of antibacterial tetracycline derivs.)

184593-35-9P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of antibacterial tetracycline derivs.)

RN 184593-35-9 HCAPLUS
CN Carbamic acid, [9-(aminocarbonyl)-7-(dimethylamino)-6,6a,7,10,10a,11-hexahydro-1,8,10a,12-tetrahydroxy-5-methyl-10,11-dioxo-2-naphthacenyl]-, methyl ester, [6aS-(6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ΙT

- L54 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2002 ACS
- AN 1995:55081 HCAPLUS
- DN 122:188050
- TI "Glycylcyclines". 3. 9-Aminodoxycyclinecarboxamides
- AU Barden, Timothy C.; Buckwalter, Brian L.; Testa, Raymond T.; Petersen, Peter J.; Lee, Ving J.
- CS Agricultural Research Division, American Cyanamid Company, Princeton, NJ,

08543-0400, USA

SO J. Med. Chem. (1994), 37(20), 3205-11 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB A series of 9-(acylamino)doxycycline derivs. has been prepd. These analogs exhibit good activity against both tetracycline-sensitive and tetracycline-resistant Gram-pos. (Staphylococcus aureus) and Gram-neg. (Escherichia coli) bacteria that are encoded with the efflux and ribosomal resistance gene factors. N,N-Dialkylglycylamido derivs. possessed the highest activity. Replacement of glycine moiety with other amino acids did not further enhance the activity.

IT 161452-37-5P 161452-40-0P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and bactericidal activity of acylaminodoxycyclines)

IT 161452-37-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and bactericidal activity of acylaminodoxycyclines)

RN 161452-37-5 HCAPLUS

CN 2-Naphthacenecarboxamide, 9-(acetylamino)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L54 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2002 ACS

AN 1994:579403 HCAPLUS

DN 121:179403

TI Preparation of 7-(substituted)-8-(substituted)-9-(substituted amino)-6-demethyl-6-deoxytetracyclines as antibiotic agents

IN Sum, Phaik Eng; Lee, Ving J.; Hlavka, Joseph J.; Testa, Raymond T.

PA American Cyanamid Co., USA

SO Eur. Pat. Appl., 181 pp. CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

$^{\circ}N$ T.	1							
PAT	TENT NO.		KIND	DATE		APPLICATION NO.	DATE	
ΕP	582810		A1	19940216		EP 1993-109850	19930621	
	R: AT,	BE,	CH, DE,	DK, ES,	FR,	GB, GR, IE, IT, LI,	LU, NL, PT,	SE
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CA	2103861		AA	19940214		CA 1993-2103861	19930811	
JΡ	06228072		A2	19940816		JP 1993-217927	19930811	
NO	9302872		A	19940214		NO 1993-2872	19930812	
ΑU	9344601		A1	19940217		AU 1993-44601	19930812	
ΑU	674524		B2	19970102				
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HU	64945		A2	19940328		ни 1993-2333	19930812	
HU	213269		В	19970428				
IL	106677		A1	19980615		IL 1993-106677	19930812	
PL	174022		В1	19980630		PL 1993-300066	19930812	
	PATEP CZ CA JP NO AU AU ZA HU HU IL	PATENT NO. EP 582810 R: AT, CZ 289195 CA 2103861 JP 06228072 NO 9302872 AU 9344601 AU 674524 ZA 9305892 HU 64945 HU 213269 IL 106677 PL 174022	PATENT NO. EP 582810 R: AT, BE, CZ 289195 CA 2103861 JP 06228072 NO 9302872 AU 9344601 AU 674524 ZA 9305892 HU 64945 HU 213269 IL 106677	PATENT NO. KIND	PATENT NO. KIND DATE	PATENT NO. KIND DATE	PATENT NO. KIND DATE APPLICATION NO. EP 582810 A1 19940216 EP 1993-109850 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, CZ 289195 B6 20011114 CZ 1993-1575 CA 2103861 AA 19940214 CA 1993-2103861 JP 06228072 A2 19940816 JP 1993-217927 NO 9302872 A 19940214 NO 1993-2872 AU 9344601 A1 19940217 AU 1993-44601 AU 674524 B2 19970102 ZA 9305892 A 19940310 ZA 1993-5892 HU 64945 A2 19940328 HU 1993-2333 HU 213269 B 19970428 IL 106677 A1 19980615 IL 1993-106677	PATENT NO. KIND DATE APPLICATION NO. DATE EP 582810 A1 19940216 EP 1993-109850 19930621 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, CZ 289195 B6 20011114 CZ 1993-1575 19930804 CA 2103861 AA 19940214 CA 1993-2103861 19930811 JP 06228072 A2 19940816 JP 1993-217927 19930811 NO 9302872 A 19940214 NO 1993-2872 19930812 AU 9344601 A1 19940217 AU 1993-44601 19930812 AU 674524 B2 19970102 ZA 9305892 A 19940310 ZA 1993-5892 19930812 HU 64945 A2 19940328 HU 1993-2333 19930812 HU 213269 B 19970428 IL 106677 A1 19980615 IL 1993-106677 19930812

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В1
                             19980630
                                              PL 1993-318908
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                        В1
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                             20000126
                                                                19940321
                                              US 1994-214992
                             19950704
     US 5430162
                        Α
                                              US 1994-352407
                                                                19941208
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                             19990323
     US 5886175
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                        Α
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PRAI US 1992-928598
                        Α
                             19920813
                        Α3
                             19930812
     IL 1993-106677
     US 1994-214992
                        В3
                             19940321
     MARPAT 121:179403
OS
GΙ
```

The title compds., e.g., I [X = halo, trifluoromethanesulfonyloxy; R, R1 = H, nitro, amino, etc.; further details on R and R1 are given], are prepd. [7S-(7.alpha.,10a.alpha.)]-[9-(Aminocarbonyl)-3-chloro-7-(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]carbamic acid Me ester (II) was prepd. from 9-azido-6-demethyl-6-deoxytetracycline hydrochloride. II in vitro showed MICs of 0.06 and 4 .mu.g/mL against Staphylococcus aureus UBMS 90-3 and Staphylococcus aureus IVES 2943 (meth. resistant), resp. The title compds. exhibit antibacterial activity against a wide spectrum of organisms including organisms which are resistant to tetracyclines.

IT 157579-07-2P 157579-18-5P 157579-22-1P 157579-23-2P 157579-26-5P 157579-28-7P 157579-29-8P 157579-30-1P 157579-31-2P 157579-36-7P 157579-37-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of, as antibiotic)

IT 157579-07-2P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as antibiotic)

RN 157579-07-2 HCAPLUS

CN Carbamic acid, [9-(aminocarbonyl)-3-chloro-7-(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

GI

```
ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2002 ACS
L54
     1993:603237
                  HCAPLUS
ΑN
     119:203237
DN
     Preparation of 7-substituted-9-substituted amino-6-demethyl-6-
ΤI
     deoxytetracyclines
     Hlavka, Joseph J.; Sum, Phaik Eng; Gluzman, Yakov; Lee, Ving J.; Ross,
ΙN
     Adma A.
     American Cyanamid Co., USA
PΑ
     Eur. Pat. Appl., 209 pp.
SO
     CODEN: EPXXDW
DT
     Patent
     English
LA
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                                                                DATE
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     CZ 284159
                        В6
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     CZ 284209
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                              19921001
      IL 1992-103320
                              19940804
                         A3
      US 1994-286096
      MARPAT 119:203237
OS
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AΒ Title compds. I (X = H2N, R1R2N wherein R1 = H, alkyl, R2 = Me, Et, Pr, Me2CH, Bu, MeCH2CHMe, Me2CHCH2, Me3C, halo; R = R4(CH2)4nCO, R4(CH2)nSO2 wherein R4 = H, C1-4 alkyl-, cyclopropyl-, cyclobutyl-, benzyl-, phenylamino, dimethyl-, diethylamino, piperidyl, morpholinyl, (substituted) cycloalkyl, (substituted) C6-10 aryl, C7-9 aralkyl, heterocyclyl, etc., n = 0-4; R' = H2N, R5R6NCH2NH wherein R5, R6 = H, C1-3alkyl, C6-10 aryl, C7-9 aralkyl, 5-6-membered heterocyclyl comprising N, O, S, Se) and a salt thereof, having activity against and including organisms resistant to tetracyclines, are prepd. To [4S-(4.alpha., 12a.alpha.)]-4,7-bis(dimethylamino)-1,4,4a,5,5a,6,11,12aoctahydro-2, 3, 10, 12, 12a-tetrahydroxy-1, 11-dioxo-2-naphthacenecarboxamide-HCl in H2SO4 was added NaNO3 to give the 9-nitro deriv. sulfate which in MeOCH2CH2OH was treated with Pd/C and H2SO4 to give the 9-amino deriv. sulfate which was reacted with NaOAc and HCO2H to give [4S-(4.alpha.,12a.alpha.)]-I (X = H2NCO, R = HCO, R' = H2N) (II). II showed in vivo activity against resistant organisms. A large no. of I was prepd. and evaluated.

IT 150231-22-4P 150231-23-5P 150251-75-5P 150251-76-6P 150251-77-7P 150251-78-8P 150521-69-0P 150521-70-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as antibacterial)

IT 150231-22-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as antibacterial)

RN 150231-22-4 HCAPLUS

CN Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, 2-(diethylamino)ethyl ester, monohydrochloride, [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

L54 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS AN 1970:455886 HCAPLUS

DN 73:55886

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TI Antibacterial alkylamino tetracyclines
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IN Zambrano, Ronald T.

PA American Cyanamid Co.

SO U.S., 4 pp.

CODEN: USXXAM

DT Patent

LA English

FAN. CNT 2

LWM.	CN1 Z					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
				~		
ΡI	US 3483251	Α	19691209	US 1967-620294	19670303	
	GB 1206439	A	19700923	GB 1967-1206439	19671215	
	FR 1550023	A	19681213	FR 1968-1550023	19680105	
	BE 709112	A	19680709	BE 1968-709112	19680109	
	NL 6800362	A	19680711	NL 1968-362	19680110	
	NL 162066	В	19791115			
	NL 162066	С	19800415			
	DE 1643767	B2	19800417	DE 1968-A57905	19680110	
	DE 1643767	C3	19810108			
	ES 352203	A1	19700201	ES 1968-352203	19680330	
	JP 52015594	B4	19770430	JP 1972-79544	19720810	
PRAI	US 1967-608264		19670110			
	US 1967-620294		19670303			

The title compds. (I) are reduced with H at atm. or superatm. pressure in AΒ the presence of a carbonyl compd. and a metal catalyst to produce biol. active 7-[mono(lower alkyl)amino]tetracyclines and 7-[di(lower alkyl)amino]tetracyclines. For example, 1 g 6-demethyltetracycline was dissolved in 9.6 ml THF and 10.4 ml methanesulfonic acid at -10.degree.. After warming the mixt. to 0.degree. a soln. of 0.86 g dibenzyl azodicarboxylate in 0.5 ml THF was added and the mixt. stirred for 2 hr at 0.degree. to yield 7-[1,2-bis(carbobenzyloxy)hydrazino]-6demethyltetracycline (II). A soln. of 1 millimole II in 90 ml 2-methoxyethanol, 1.5 ml 40% aq. $\rm H2CO$ and 300 mg 10% $\rm Pd$ -C was hydrogenated at room temp. to give 7-dimethylamino-6-demethyltetracycline. Similarly 7-[1,2-bis(carbobenzyloxy)hydrazino]-6-demethyl-6-deoxytetracycline and 7-dimethylamino-.alpha.-6-deoxy-5-hydroxytetracycline were prepd. Other starting tetracyclines prepd. were 7-[1,2-bis(carbobenzyloxy)hydrazino]-6demethyl-6-deoxytetracycline and 7-[1,2 - bis(carbobenzyloxy)hydrazino] -11a-chloro-6-demethyl-6-deoxytetracycline. I are biol. active and possess broad spectrum antibacterial activity.

IT 22229-68-1P 22229-72-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 22229-68-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 22229-68-1 HCAPLUS

CN Bicarbamic acid, [8-carbamoyl-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, dibenzyl ester (8CI) (CA INDEX NAME)

L54

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ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2002 ACS
AN
      1969:37557 HCAPLUS
DN
      70:37557
ΤI
      7-[1,2-Bis(substituted)hydrazino]tetracyclines
IN
      Zambrano, Ronald T.
PΑ
     American Cyanamid Co.
SO
     U.S., 5 pp.
     CODEN: USXXAM
DT
     Patent
LA
     English
FAN.CNT 2
     PATENT NO.
                       KIND DATE
                                             APPLICATION NO.
                                                              DATE
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                            -----
                                                              -----
ΡI
     US 3403179
                       Α
                             19680924
                                             US 1967-608264
                                                               19670110
     GB 1206439
                       Α
                             19700923
                                             GB 1967-1206439
                                                              19671215
     FR 1550023
                       Α
                             19681213
                                             FR 1968-1550023
                                                              19680105
     BE 709112
                       Α
                             19680709
                                             BE 1968-709112
                                                               19680109
     NL 6800362
                       A
                             19680711
                                             NL 1968-362
                                                              19680110
     NL 162066
                       В
                             19791115
     NL 162066
                       С
                             19800415
     DE 1643767
                       B2
                             19800417
                                             DE 1968-A57905
                                                              19680110
     DE 1643767
                       C3
                             19810108
     ES 352203
                       A1
                             19700201
                                             ES 1968-352203
                                                              19680330
     JP 52015594
                       B4
                             19770430
                                             JP 1972-79544
                                                              19720810
PRAI US 1967-608264
                             19670110
     US 1967-620294
                             19670303
GI
     For diagram(s), see printed CA Issue.
AΒ
     6-Demethyl-6-deoxytetracycline (3.84 g.) was dissolved in a mixt. of 7.7
     cc. tetrahydrofuran and 69 cc. MeSO3H, and the soln. cooled to
     0-5.degree.. A soln. of 3.32 g. PhCH2O2CN:NCO2CH2Ph in 3.1 cc.
     tetrahydrofuran was added dropwise, and the mixt. stirred 10 min. to give
     5.55 g. I (R = PhCH2O2C) (II). II (7 g.) was reduced with 3.5 g 50% \bar{P}d-C
     and 136 ml. N H2SO4-MeOH for 4 hrs. at 20 psi. H to give
     7-amino-6-demethyl-6-deoxytetracycline. Redn. in the presence of H2CO
     gave the 7-dimethylamino analog. Also prepd. were I (R = EtO2C) and I (R = H2NCO). Also prepd. were 7-(1,2-dicarbethoxyhydrazino)-.beta.-6-deoxy-5-
     hydroxytetracycline, 7-(1,2-dicarbethoxyhydrazino)-.beta.-6-
     deoxytetracycline, and 7-[1,2-bis(carbobenzyloxy)hydrazino]-11a-chloro-6-
     demethyl-6-deoxytetracycline. Spectral data are given for many of the
     compds.
IT
     22229-68-1P 22229-71-6P 22229-72-7P
     22229-73-8P 22351-64-0P 22351-65-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
     22229-68-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     22229-68-1 HCAPLUS
CN
     Bicarbamic acid, [8-carbamoyl-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-
     octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, dibenzyl ester
     (8CI) (CA INDEX NAME)
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=> d 153 bib abs hitrn fhitstr tot
     ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ΑN
     2002:51420 HCAPLUS
DN
     136:102232
     Preparation of 7-substituted tetracycline derivatives for pharmaceutical
TI
     use as antibacterial agents
IN
     Nelson, Mark L.; Frechette, Roger; Viski, Peter;
     Ismail, Mohamed; Bowser, Todd; Bhatia, Beena;
     Messersmith, David; McIntyre, Laura; Koza, Darrell; Rennie, Glen; Sheahan,
     Paul; Hawkins, Paul; Verma, Atul; Warchol, Tad; Bandarage, Upul
PA
     Trustees of Tufts College, USA; Paratek Pharmaceuticals,
     Inc.
SO
     PCT Int. Appl., 97 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
    WO 2002004407
                       A2
                                           WO 2001-US20766
                            20020117
                                                            20010629
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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PΙ CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, ТJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG PRAI US 2000-216760 Ρ 20000707 US 2001-275576 Ρ 20010313 GΙ

AΒ 7-Substituted tetracycline derivs., such as I [R7 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl,

alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prepd. for therapeutic use as antibacterial agents. Thus, 7-phenylsancycline I (R7 = Ph) was prepd. in 42% yield by arom. coupling reaction of 7-iodosancycline I (R7 = iodo) with PhB(OH)2 using Pd(OAc)2 and Na2CO3 in MeOH under an argon atm. at r.t. for 2 h. The prepd. tetracycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus.

IT 365277-44-7P 365277-45-8P 389625-03-0P 389625-12-1P 389625-13-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

IT 365277-44-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

RN 365277-44-7 HCAPLUS

CN Carbamic acid, [(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, 4-methoxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L53 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
- AN 2002:51419 HCAPLUS
- DN 136:102231
- TI Preparation of 9-substituted minocycline derivatives for pharmaceutical use as antibacterial agents
- IN Nelson, Mark L.; Frechette, Roger; Viski, Peter;
 Ismail, Mohamed; Bowser, Todd; Dumornay, Jimmy; Rennie,
 Glen; Liu, Gui; Koza, Darrell; Sheahan, Paul; Stapleton, Karen; Hawkins,
 Paul; Bhatia, Beena; Verma, Atul; McIntyre, Laura; Warchol, Tad
- PA Trustees of Tufts College, USA; Paratek Pharaceuticals,
- SO PCT Int. Appl., 57 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2002004406 A2 20020117 WO 2001-US20721 20010629

PI WO 2002004406 A2 20020117 WO 2001-US20721 20010629 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-216659 P 20000707
US 2001-275621 P 20010313
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AB 9-Substituted minocycline derivs., such as I [R9 = NO2, N:S, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prepd. for therapeutic use as antibacterial agents. Thus, minocycline deriv. I (R9 = CH2NHCONHC6H4-4-OCF3) was prepd. in 37% yield by reaction of the trihydrochloride salt of 9-(aminomethyl)minocycline I (R9 = CH2NH2) and F3CO-4-C6H4NCO using Et3N in DMF at 25.degree. for 2 h. The prepd. minocycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus. IT 365277-07-2P 365277-29-8P

Ι

365277-07-2P 365277-28-7P 365277-29-8P 365277-36-7P 365277-38-9P 365277-46-9P 365277-47-0P 365277-48-1P 365277-49-2P 365277-50-5P 365277-51-6P 365277-52-7P 365277-53-8P 365277-54-9P 365277-55-0P 365277-56-1P 365277-57-2P 365277-58-3P 365277-62-9P 365277-61-8P 365277-62-9P 365277-63-0P 365277-64-1P 365277-65-2P 389139-81-5P 389139-82-6P 389139-93-9P 389139-86-0P 389139-92-8P 389139-93-9P 389139-94-0P 389139-95-1P 389139-96-2P 389139-97-3P 389139-98-4P 389139-99-5P 389140-00-5P 389140-01-6P 389140-02-7P 389140-03-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 9-substituted minocycline derivs. for pharmaceutical use as antibacterial agents)

IT 365277-07-2P

RN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 9-substituted minocycline derivs. for pharmaceutical use as antibacterial agents)

365277-07-2 HCAPLUS

CN Carbamic acid, [(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]-, 2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

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L53 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
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AN 2001:747739 HCAPLUS

DN 135:288637

TI Preparation of 7-and 9-carbamate, urea, thiourea, thiocarbamate, and heteroaryl-amino substituted tetracycline derivatives for pharmaceutical use as antibiotics

IN Nelson, Mark L.; Levy, Stuart B.; Prechette, Roger; Bowser, Todd E.; Ismail, Mohamed Y.

PA Trustees of Tufts College, USA

SO PCT Int. Appl., 88 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

ran.eni i							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	WO 2001074761		20011011	WO 2001-US10342	20010331		
	W: AE, AG	, AL, AM,	, AT, AU, AZ,	BA, BB, BG, BR, BY,	BZ, CA, CH, CN,		
	CO, CR	, CU, CZ,	, DE, DM, DZ,	EE, ES, FI, GB, GD,	GE, GH, GM, HR.		
	HU, ID	, IL, IN,	, IS, JP, KE,	KG, KP, KR, KZ, LC,	LK, LR, LS, LT,		
	LU, LV	, MA, MD,	, MG, MK, MN,	MW, MX, MZ, NO, NZ,	PL, PT, RO, RU.		
	SD, SE	, SG, SI,	, SK, SL, TJ,	TM, TR, TT, TZ, UA,	UG, VN, YU, ZA, ZW		
	RW: GH, GM	KE, LS,	, MW, MZ, SD,	SL, SZ, TZ, UG, ZW,	AT, BE, CH, CY,		
	DE, DK	ES, FI,	, FR, GB, GR,	IE, IT, LU, MC, NL,	PT, SE, TR, BF.		
	BJ, CF	CG, CI,	CM, GA, GN,	GW, ML, MR, NE, SN,	TD, TG		
PRAI	US 2000-193879	P	20000331		,		
	US 2000-193972	P	20000331				
os	MARPAT 135:288	537					
GI							

Tetracycline derivs., such as I [R5 = H, OH, acyloxy, etc.; R6 = H, Me, alkyl, etc.; R7, R9 = arylamino, urea, thiourea, carbamate, thiocarbamate, etc.; R8 = H, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, etc.], were prepd. for pharmaceutical use as antibiotics. Thus, doxycycline deriv. I (R5 = OH, R6 = Me, R7 = R8 = H, R9 = 1-naphthylaminocarbonylamino) was prepd. by nitration of doxycycline with potassium nitrate, Pd/C catalyzed hydrogenation of the nitrate to form 9-aminodoxycycline I (R5 = OH, R6 = Me, R7 = R8 = H, R9 = NH2) followed by formation of the desired urea by reaction of 9-aminodoxycycline with 1-naphthylisocyanate. The prepd. tetracycline derivs. were tested for efficacy against common bacterial strains, such as E. coli, S. aureus, E.

Ι

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hirae, and E. faecalis.
ΙT
     365277-08-3P
     RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
     SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepn. of 7-and 9-carbamate, urea, thiourea, thiocarbamate, and
        heteroaryl-amino substituted tetracycline derivs. for pharmaceutical
        use as antibiotics)
ΙT
     161452-37-5P 365276-98-8P 365276-99-9P
     365277-00-5P 365277-01-6P 365277-02-7P
     365277-03-8P 365277-04-9P 365277-05-0P
     365277-06-1P 365277-07-2P 365277-09-4P
     365277-15-2P 365277-16-3P 365277-19-6P
     365277-20-9P 365277-21-0P 365277-22-1P
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     365277-34-5P 365277-35-6P 365277-36-7P
     365277-38-9P 365277-44-7P 365277-45-8P
     365277-46-9P 365277-47-0P 365277-48-1P
     365277-49-2P 365277-50-5P 365277-51-6P
     365277-52-7P 365277-53-8P 365277-54-9P
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     365277-89-0P 365277-90-3P 365277-91-4P
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     365278-09-7P 365278-10-0P 365278-11-1P
     365278-12-2P 365278-13-3P 365278-14-4P
     365278-15-5P 365280-21-3P
     RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (prepn. of 7-and 9-carbamate, urea, thiourea, thiocarbamate, and
        heteroaryl-amino substituted tetracycline derivs. for pharmaceutical
        use as antibiotics)
IT
     365277-08-3P
     RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
     SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepn. of 7-and 9-carbamate, urea, thiourea, thiocarbamate, and
        heteroaryl-amino substituted tetracycline derivs. for pharmaceutical
        use as antibiotics)
     365277-08-3 HCAPLUS
RN
     Carbamic acid, [[[(5R,5aR,6S,6aR,7S,10aS)-9-(aminocarbonyl)-7-
CN
     (dimethylamino) -5, 5a, 6, 6a, 7, 10, 10a, 12-octahydro-1, 6, 8, 10a, 11-pentahydroxy-
     5-methyl-10,12-dioxo-2-naphthacenyl]amino]thioxomethyl]-,
     9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)
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RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil reg FILE 'REGISTRY' ENTERED AT 14:13:47 ON 11 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9 DICTIONARY FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

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1
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                389140-02-7
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                             REGISTRY
          RN
                389139-99-5
          RN
                389139-98-4 REGISTRY
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                 389139-92-8
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                 389139-83-7
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                 389139-82-6
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           RN
                 389139-81-5
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           RN
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21
           RN
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                 365278-12-2
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25
           RN
                 365278-11-1
                                REGISTRY
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L48 ANSWER 1 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 389625-13-2 REGISTRY

CN INDEX NAME NOT YET ASSIGNED

FS STEREOSEARCH

MF C26 H31 N3 O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:102232

L48 ANSWER 4 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 389140-03-8 REGISTRY

CN Carbamic acid, [[(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]methyl]-, pentyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H40 N4 O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:102231

L48 ANSWER 10 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 389139-97-3 REGISTRY

CN Carbamic acid, [[(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]methyl]-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H31 C13 N4 O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:102231

L48 ANSWER 15 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 389139-92-8 REGISTRY

CN Carbamic acid, [[(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]methyl]-, hexyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H42 N4 O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:102231

L48 ANSWER 20 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365280-21-3 REGISTRY

CN Carbamic acid, [(5aR, 6aS, 7S, 10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-

naphthacenyl]-, 1-methylethenyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H32 N4 O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 21 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365278-15-5 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro- $3, 10, 12, 12 \\ a-tetra \\ hydroxy-6-methyl-7-[[(1-naphthalenylamino)thioxomethyl]] \\ amount \\ amount$ ino]-1,11-dioxo-5-(1-oxopropoxy)-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C36 H36 N4 O9 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 30 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365278-06-4 REGISTRY

CN Carbamothioic acid, [(6aS,10S,10aR,11S,11aR,12R)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9,11-pentahydroxy-12-methyl-5,7-dioxo-1-naphthacenyl]-, O-(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C37 H35 N3 O9 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 40 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN **365277-87-8** REGISTRY

CN Carbamic acid, [(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]-, pentyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H38 N4 O9

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 50 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365277-69-6 REGISTRY

CN 2-Naphthacenecarboxamide, 4,7-bis(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-9-[[[(3-methylbutyl)amino]carbonyl]amino]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H39 N5 O8

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 60 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN **365277-58-3** REGISTRY

CN Carbamic acid, [(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]-, 4-bromophenyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H31 Br N4 O9

SR CA

LC STN Files: CA, CAPLUS

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1:

1: 136:102231

REFERENCE

2: 135:288637

L48 ANSWER 70 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365277-48-1 REGISTRY

CN 2-Naphthacenecarboxamide, 4,7-bis(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-9-[[[(4-nitrophenyl)amino]carbonyl]amino]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H32 N6 O10

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE

1: 136:102231

REFERENCE

2: 135:288637

L48 ANSWER 80 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN **365277-31-2** REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-[[[[4-[[5-(dimethylamino)-2-naphthalenyl]sulfonyl]phenyl]amino]thioxomethyl]amino]1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C41 H41 N5 O10 S2

SR CA

LC STN Files: CA, CAPLUS

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 90 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 365277-20-9 REGISTRY

CN 2-Naphthacenecarboxamide, 9-[[[(4-chlorophenyl)sulfonyl]amino]carbonyl]amino]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H29 C1 N4 O11 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 100 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN **365277-03-8** REGISTRY

CN Carbamic acid, [(5R,5aR,6S,6aR,7S,10aS)-9-(aminocarbonyl)-7-(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,6,8,10a,11-pentahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

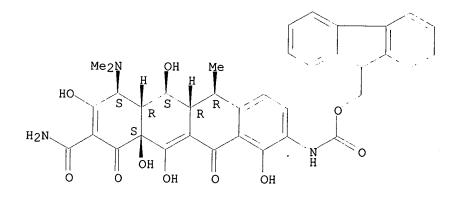
FS STEREOSEARCH

MF C37 H35 N3 O10

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:288637

L48 ANSWER 106 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 184593-69-9 REGISTRY

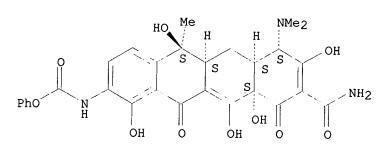
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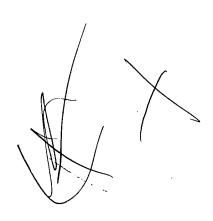
FS STEREOSEARCH

MF C29 H29 N3 O10

SR CA

LC STN Files: CA, CAPLUS, USPATFULL





^{**}PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:31223

L48 ANSWER 110 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 184593-35-9 REGISTRY

CN Carbamic acid, [9-(aminocarbonyl)-7-(dimethylamino)-6,6a,7,10,10a,11-hexahydro-1,8,10a,12-tetrahydroxy-5-methyl-10,11-dioxo-2-naphthacenyl]-, methyl ester, [6aS-(6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H25 N3 O9

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:31223

L48 ANSWER 112 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 161452-40-0 REGISTRY

CN Carbamic acid, [9-(aminocarbonyl)-7-(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,6,8,10a,11-pentahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, methyl ester, [5R-(5.alpha.,5a.alpha.,6.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H27 N3 O10

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:188050

L48 ANSWER 114 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 157579-37-8 REGISTRY

CN Carbamic acid, [9-(aminocarbonyl)-3-bromo-7-(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]-, methyl ester, [5aR-(5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H24 Br N3 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 121:179403

L48 ANSWER 120 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 157579-26-5 REGISTRY

CN Carbamic acid, [8-(aminocarbonyl)-2-chloro-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, methyl ester, [6aS-(6a.alpha.,10.alpha.,10a.alpha.,11a.alpha.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H24 C1 N3 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 121:179403

L48 ANSWER 125 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 150521-70-3 REGISTRY

CN Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, ethenyl ester, [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]-, sulfate (salt) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H32 N4 O9 . x H2 O4 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 150251-77-7 CMF C27 H32 N4 O9

Absolute stereochemistry.

CM 2

CRN 7664-93-9 CMF H2 O4 S

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:203237

L48 ANSWER 131 OF 139 REGISTRY COPYRIGHT 2002 ACS

RN 150231-23-5 REGISTRY

CN Carbamic acid, [9-(aminocarbonyl)-4,7-bis(dimethylamino)-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-5-methyl-10,12-dioxo-2-naphthacenyl]-, 2-propenyl ester, monohydrochloride, [5R-(5.alpha.,5a.alpha.,6a.alpha.,7.alpha.,10a.alpha.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H34 N4 O9 . C1 H

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CRN (150251-78-8)

Absolute stereochemistry.

● HCl

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

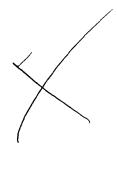
REFERENCE 1: 119:203237

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RN 28268-56-6 REGISTRY

CN 1,2-Hydrazinedicarboxylic acid, 1-[8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9,12-pentahydroxy-5,7-dioxo-1-naphthacenyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

MF C37 H36 N4 O12



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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RN 22351-65-1 REGISTRY

CN Biurea, 3-[8-carbamoyl-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (8CI) (CA INDEX NAME)

MF C23 H26 N6 O9

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 70:37557

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RN 22229-73-8 REGISTRY

CN Bicarbamic acid, [8-carbamoyl-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, diethyl ester (8CI) (CA INDEX NAME)

MF C27 H32 N4 O11

CI COM

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 70:37557

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RN 22229-68-1 REGISTRY

CN Bicarbamic acid, [8-carbamoyl-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, dibenzyl ester (8CI) (CA INDEX NAME)

MF C37 H36 N4 O11

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 73:55886

REFERENCE 2: 70:37557